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Solving moment and polynomial optimization problems on Sobolev spaces^{*}

Didier Henrion^{1,2}, Alessandro Rudi

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Abstract

Using standard tools of harmonic analysis, we state and solve the problem of moments for positive measures supported on the unit ball of a Sobolev space of multivariate periodic trigonometric functions. We describe outer and inner semidefinite approximations of the cone of Sobolev moments. They are the basic components of an infinite-dimensional moment-sums of squares hierarchy, allowing to solve numerically non-convex polynomial optimization problems on infinite-dimensional Sobolev spaces, with global convergence guarantees.

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1 Introduction

The *moment-SOS hierarchy*, also known as the Lasserre hierarchy, was originally introduced in the early 2000s to solve globally finite-dimensional *polynomial optimization problems* (POP) [19, 21, 8, 26]. Then it was extended to polynomial differential equations and their optimal control, see [16] for a recent overview of applications and more references. The main technical ingredients on which the moment-SOS hierarchy relies are sums of squares (SOS) representations of positive polynomials (the so-called Positivstellensätze) [22] and its dual problem of moments [29] providing conditions satisfied by moments of a positive measure supported on a finite-dimensional set. These conditions are truncated to finite degrees, yielding a converging hierarchy of semidefinite optimization problems of increasing size that can be solved numerically using interior-point algorithms [24, 6].

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After more than two decades of research in polynomial optimization, the application range of the moment-SOS hierarchy is now being extended to challenging nonconvex nonlinear optimization problems formulated on infinite-dimensional functional spaces, e.g. problems of calculus of variations or partial differential equations. The moment-SOS hierarchy has been recently extended to reproducible kernel Hilbert spaces for polynomial optimization [28] or optimal transport [23]. Measures supported on infinite-dimensional spaces arise naturally as relaxed controls for infinite-dimensional optimization [11]. Ambrosio's superposition principle [2] whose finite-dimensional Euclidean version was used in [15] to prove convergence of the moment-SOS hierarchy for approximating the region of attraction of polynomial differential equations, has been extended to infinite-dimensional Hilbert or Banach spaces [3]. Measures on infinite-dimensional spaces are also used in fluid dynamics, see e.g. [13] or more recently [27] which presents itself as an infinite-dimensional extension of the finite-dimensional SOS setup of [32]. The solution of the moment problem for measures supported on infinite-dimensional spaces is more technically involved than its finite-dimensional counterpart, see [18, 30] and references therein. The recent reference [14] shows however that the heat equation with polynomial nonlinearities can be solved numerically with the infinite-dimensional moment-SOS hierarchy, with convergence guarantees provided by a recent solution of the moment problem on nuclear spaces [17].

The present paper aims at contributing to the numerical solution of the *infinite-dimensional* moment problem in a functional analytic framework which makes its analysis as well as its numerical implementation as simple as possible. We use basic tools from harmonic analysis to state and solve the moment problem on the Sobolev space of periodic multivariate trigonometric functions. This allows us to construct an infinite-dimensional moment-SOS hierarchy to solve various kinds of *Sobolev POPs*, namely non-convex POPs on Sobolev spaces, with global convergence guarantees.

In order to keep this paper as short and elementary as possible, we do not describe here potential applications of the moment-SOS hierarchy for solving non-linear calculus of variations problems, or optimal control problem involving non-linear partial differential equations. Such applications are certainly very promising, and they will be reported in further communications.

The outline of the paper is as follows. In Section 2 we state our Sobolev moment problem. In Section 3 we reformulate our Sobolev moment problem as a moment problem in the Fourier coefficients. In Section 4 we propose inner and outer semidefinite approximations of the Sobolev moment cone. This allows us to solve different types of Sobolev POPs with an infinite-dimensional moment-SOS hierarchy in Section 5. Concluding remarks and potential extensions are mentioned in Sections 6 and 7.

2 Sobolev moment problem

Consider the space of Sobolev functions on the n -dimensional unit torus T^n whose derivative up to order m are square integrable:

$$H^m(T^n) := \{f : T^n \rightarrow \mathbb{C} : \|f\|_{H^m(T^n)}^2 < \infty\}$$

where the norm is defined as:

$$\|f\|_{H^m(T^n)}^2 := \sum_{|a| \leq m} \int_{T^n} \|D^a f(x)\|^2 dx$$

with $a \in \mathbb{N}^n$, $|a| = \sum_{i=1}^n a_i$ and $D^a = \frac{\partial^{|a|}}{\partial x_1^{a_1} \dots \partial x_n^{a_n}}$.

Let $c_0(\mathbb{Z}^n)$ denote the set of sequences consisting of a finite number of elements of \mathbb{Z}^n , allowing repetitions. Let us consider the closed bounded unit ball of $H^m(T^n)$

$$B := \{f \in H^m(T^n) : \|f\|_{H^m(T^n)} \leq 1\}.$$

Let μ be a measure supported on B , and let $\mathbf{a} \in c_0(\mathbb{Z}^n)$. The *moment* of μ of index \mathbf{a} is defined as:

$$y_{\mathbf{a}} := \int_B m_{\mathbf{a}}(f) d\mu(f)$$

with

$$m_{\mathbf{a}}(f) := \prod_{a \in \mathbf{a}} \langle f, e_a \rangle$$

the *monomial* of f of index \mathbf{a} , for the scalar product

$$\langle f, e_a \rangle_{H^m(T^n)} := \int_{T^n} f(x) e_a(x) dx, \quad e_a(x) := e^{-2\pi i \langle a, x \rangle_{\mathbb{R}^n}}. \quad (1)$$

Note that since $\mathbf{a} \in c_0(\mathbb{Z}^n)$, it follows that $m_{\mathbf{a}}(f)$ is the product of finitely many coefficients. The *algebraic degree* is $d_{\mathbf{a}} := \#\mathbf{a}$, the cardinality of \mathbf{a} , i.e. the number of terms in the product defining $m_{\mathbf{a}}(f)$. The *harmonic degree* is the integer $\delta_{\mathbf{a}} := \max_{a \in \mathbf{a}} \max_{i=1, \dots, n} |a_i|$.

Example 1. Let $n = 2$. The empty set $\mathbf{a} = \{\} = \emptyset$ indexes the mass $\int_B d\mu(f)$, $\mathbf{a} = \{(0, 0)\}$ indexes the first degree moment $\int_B \langle f, e_{(0,0)} \rangle d\mu(f)$, $\mathbf{a} = \{(0, 0), (0, 0)\}$ indexes the second degree moment $\int_B \langle f, e_{(0,0)} \rangle^2 d\mu(f)$, $\mathbf{a} = \{(1, 0), (0, -1), (0, -1)\}$ indexes the third degree moment $\int_B \langle f, e_{(1,0)} \rangle \langle f, e_{(0,-1)} \rangle^2 d\mu(f)$, etc.

We can now state the problem addressed in this paper.

Sobolev moment problem: Let $N \in \mathbb{N}$. Given an index set $A \in c_0(\mathbb{Z}^n)^N$ and a vector $(y_{\mathbf{a}})_{\mathbf{a} \in A} \in \mathbb{C}^N$, find a measure μ on B such that

$$y_{\mathbf{a}} = \int_B m_{\mathbf{a}}(f) d\mu(f), \text{ for all } \mathbf{a} \in A. \quad (2)$$

Since we defined a monomial in Sobolev space, we can also define a *polynomial* p as a linear combinations of monomials:

$$p(f) := \sum_{\mathbf{a} \in \text{spt } p} p_{\mathbf{a}} m_{\mathbf{a}}(f)$$

where the support $\text{spt } p \subset c_0(\mathbb{Z}^n)$ is the index set of coefficients in the monomial basis, the algebraic degree is $d(p) := \max_{\mathbf{a} \in \text{spt } p} d_{\mathbf{a}}$ and the harmonic degree is $\delta(p) := \max_{\mathbf{a} \in \text{spt}(p)} \delta_{\mathbf{a}}$.

3 Fourier embedding

Let us reformulate our moment problem in the space of Fourier coefficients. The following results are classical [1].

Define the Fourier transform $F : L^2(T^n) \rightarrow \ell_2(\mathbb{Z}^n)$, $f \mapsto c$ where $c := (c_a)_{a \in \mathbb{Z}^n}$ and $c_a := \langle f, e_a \rangle_{H^m(T^n)}$ is the Fourier coefficient of index $a \in \mathbb{Z}^n$ of f . The adjoint of F is the inverse Fourier transform $F^* : \ell_2(\mathbb{Z}^n) \rightarrow L^2(T^n)$, $c \mapsto f = \langle c, e \rangle_{\ell^2} = \sum_{a \in \mathbb{Z}^n} c_a e_{-a}$ where $e := (e_a)_{a \in \mathbb{Z}^n}$.

Proposition 1. *The space $H^m(T^n)$ admits an equivalent norm in terms of the Fourier basis: $\|f\|_{H^m(T^n)}^2 = \sum_{a \in \mathbb{Z}^n} w_a c_a^2$, $c = Ff$ and $w_a := (1 + \langle a, a \rangle)^m$, $a \in \mathbb{Z}^n$.*

Define the diagonal operator $W : \ell_2(\mathbb{Z}^n) \rightarrow \ell_2(\mathbb{Z}^n)$, $(c_a)_{a \in \mathbb{Z}^n} \mapsto (c_a w_a)_{a \in \mathbb{Z}^n}$.

Proposition 2. *The space $H^m(T^n)$ is isomorphic to ℓ_2 via the operator F^*W . Namely, defining $f_c := F^*c$ for any $c \in \ell_2(\mathbb{Z}^n)$, we have*

$$H^m(T^n) = \{f_c : c \in \ell_2(\mathbb{Z}^n)\}, \quad \|f_c\|_{H^m(T^n)}^2 = \|c\|_W^2 := \sum_{k \in \mathbb{Z}^n} w_k c_k^2.$$

From this it follows that for any $f \in H^m(T^n)$ there exists a unique $c \in \ell_2(\mathbb{Z}^n)$ such that $f = F^*Wc$. Now define the set of Fourier coefficients

$$E := \{Ff : f \in B\} \subset \ell_2(\mathbb{Z}^n).$$

Proposition 3. *E is compact. Moreover B is one to one to E and in particular $B = \{F^*c : c \in E\}$.*

Proof. E is the linear image of the closed unit ball B of $H^m(T^n)$. By definition $E = \{FF^*Wc : c \in \ell_2(\mathbb{Z}^n)\} = W\ell_2(\mathbb{Z}^n)$. The compactness of E is obtained by noting that $1/w_a \rightarrow 0$ as $|a| \rightarrow \infty$. \square

Geometrically, E is an ellipsoid in the space of Fourier coefficients, with coordinates bounded by $1/w_a$ for any $a \in \mathbb{Z}^n$.

Let

$$\nu := F_{\#}^* \mu \tag{3}$$

denote the pushforward measure of μ through F^* . For any $\mathbf{a} \in c_0(\mathbb{Z}^n)$, the moment $y_{\mathbf{a}}$ of μ can then be expressed as a moment of ν in the space of Fourier coefficients:

$$y_{\mathbf{a}} = \int_B m_{\mathbf{a}}(f) d\mu(f) = \int_E c^{\mathbf{a}} d\nu(c), \quad c^{\mathbf{a}} := \prod_{a \in \mathbf{a}} c_a. \quad (4)$$

Proposition 4. *There is a solution to the Sobolev moment problem (2) on the ball B if and only if there is a solution to the Fourier moment problem*

$$y_{\mathbf{a}} = \int_E c^{\mathbf{a}} d\nu(c), \quad \forall \mathbf{a} \in A \quad (5)$$

on the ellipsoid E .

Proof. Since the ball B is one to one to the ellipsoid E and in particular $B = \{F^*c : c \in E\}$, then for any $f \in B$ there exists a $c \in E$ s.t.

$$\langle f, e_a \rangle_{H^m(T^n)} = \langle F^*c, e_a \rangle_{\ell_2} = w_a c_a.$$

Conversely, for any $f \in B$ there exists a unique $c \in E$ such that $f = F^*Wc$. \square

4 Semidefinite approximations of the Sobolev moment cone

Given an index set $A \subset c_0(\mathbb{Z}^n)^N$, let us define the cone of Sobolev moments

$$C(A) := \{(y_{\mathbf{a}})_{\mathbf{a} \in A} : y_{\mathbf{a}} = \int_B m_{\mathbf{a}}(f) d\mu(f) \text{ for some } \mu \text{ supported on } B\} \subset \mathbb{C}^N.$$

The Sobolev moment problem introduced previously is the membership oracle for $C(A)$, namely: does a given vector belong to this cone? Despite being convex and finite-dimensional, the cone $C(A)$ is difficult to manipulate directly. It must be approximated by linear sections and projections of a finite-dimensional convex cone on which optimization can be carried out efficiently, namely the semidefinite cone.

4.1 Outer approximations

We can construct outer approximations, or relaxations of $C(A)$, by projecting finite-dimensional spectrahedra (i.e. linear sections of the semidefinite cone) of increasing size. Let $\Pi_A : \ell_2(\mathbb{Z}^n) \rightarrow \mathbb{C}^N, y \mapsto (y_{\mathbf{a}})_{\mathbf{a} \in A}$ denote the projection map onto the subspace indexed by A . We use the Fourier embedding of the previous section to express the Sobolev moment cone as the Fourier moment cone

$$C(A) = \{(y_{\mathbf{a}})_{\mathbf{a} \in A} : y_{\mathbf{a}} = \int_E c^{\mathbf{a}} d\nu(c) \text{ for some } \nu \text{ supported on } E\} \subset \mathbb{C}^N.$$

Let $\mathbb{C}[c]$ denote the set of complex polynomials of the indeterminate c . Elements of $\mathbb{C}[c]$ can be expressed as linear combinations of monomials $p(c) = \sum_{\mathbf{a} \in \text{spt}(p)} p_{\mathbf{a}} c^{\mathbf{a}}$ with

algebraic degree $d(p) := \max_{\mathbf{a} \in \text{spt}(p)} d_{\mathbf{a}}$ and harmonic degree $\delta(p) := \max_{\mathbf{a} \in \text{spt}(p)} \delta_{\mathbf{a}}$. We are particularly interested in *Hermitian polynomials*, i.e. elements of $\mathbb{C}[c]$ with values in \mathbb{R} .

Given $r, \rho \in \mathbb{N}$, let $\mathbb{C}[c]_{r,\rho} := \{p \in \mathbb{C}[c] : d(p) \leq r, \delta(p) \leq \rho\}$ and define the cone of Hermitian polynomial sums of squares

$$\Sigma_{r,\rho} := \left\{ \sum_k q_k^* q_k : q_k \in \mathbb{C}[c]_{r,\rho} \right\}$$

and the quadratic module

$$Q_{r,\rho} := \{p = s_0 + s_1(1 - \|c\|_W^2) : s_0, s_1 \in \Sigma_{r,\rho}\}.$$

Given a sequence $y = (y_{\mathbf{a}})_{\mathbf{a} \in \mathbb{Z}^n} \in \ell_2(\mathbb{Z}^n)$, define the linear functional $\ell_y : \mathbb{C}[c] \rightarrow \mathbb{C}$, $p(c) := \sum_{\mathbf{a}} p_{\mathbf{a}} c^{\mathbf{a}} \mapsto \ell_y(p) := \sum_{\mathbf{a}} p_{\mathbf{a}} y_{\mathbf{a}}$. Let $d_A := \max_{\mathbf{a} \in A} d_{\mathbf{a}}$ denote the algebraic degree of A , and let $\rho_A := \max_{\mathbf{a} \in A} \delta_{\mathbf{a}}$ denote the harmonic degree of A . Finally, define the following cone

$$C_{r,\rho}^{\text{out}}(A) := \Pi_A \{y : \ell_y(p) \geq 0 \text{ for all } p \in Q_{r,\rho}\}.$$

Proposition 5. *For any $r \geq d_A$ and $\rho \geq \rho_A$, $C_{r,\rho}^{\text{out}}(A)$ is a semidefinite representable outer approximation of $C(A)$.*

Proof. To prove the outer approximation claim, let us a vector $y \in C(A)$ and let us prove that $y \in C_{r,\rho}^{\text{out}}(A)$. Since $y \in C(A)$, from Proposition 4 there exists a measure ν supported on E such that $y_{\mathbf{a}} = \int_E c^{\mathbf{a}} d\nu(c)$. In particular, for any real valued polynomial $p(c) = \sum_{\mathbf{a}} p_{\mathbf{a}} c^{\mathbf{a}}$ which is non-negative on E , vector y is such that $\ell_y(p) = \sum_{\mathbf{a}} p_{\mathbf{a}} y_{\mathbf{a}} = \sum_{\mathbf{a}} p_{\mathbf{a}} \int_E c^{\mathbf{a}} d\nu(c) = \int_E p(c) d\nu(c)$ is nonnegative. In particular this holds for polynomials of the form $p = q_0^* q_0 + q_1^* q_1 (1 - \|c\|_W^2)$, and hence $y \in C_{r,\rho}^{\text{out}}(A)$.

To prove the semidefinite representability claim, observe that the quadratic form $\ell_y : \mathbb{C}[c] \rightarrow \mathbb{R}, q \mapsto \ell_y(q^* q)$ can be expressed as a Hermitian matrix linear in y . Non-negativity of the quadratic form is therefore equivalent to positive semidefiniteness of a matrix which is linear in y , i.e. as a linear matrix inequality. Testing non-negativity of $\ell_y(p)$ for all $p \in Q_{r,\rho}$ amounts to testing non-negativity of $q \mapsto \ell_y(q^* q)$ and $q \mapsto \ell_y((1 - \|c\|_W^2) q^* q)$. These quadratic forms are finite dimensional, so it follows that testing membership in $C_{r,\rho}^{\text{out}}(A)$ amounts to testing membership in the projection of a spectrahedron, a finite-dimensional linear slice of the semidefinite cone. \square

Proposition 6. $\overline{C_{\infty,\infty}^{\text{out}}}(A) = C(A)$.

Proof. According to Putinar's Positivstellensatz – see e.g. [21, Thm. 3.20] or [19, Thm. 2.14], every polynomial p which is strictly positive on E can be written as $p = s_0 + s_1(1 - \|c\|_W^2)$ for s_0 and s_1 sums of Hermitian squares of polynomials. So the closure of the quadratic module $Q_{r,\rho}$ coincides with the cone of polynomials that are non-negative on E . \square

Proposition 7. *For any $r \geq r_A$ and $\rho \geq \rho_A$, the Hausdorff distance d_H between $C(A)$ and $C_{r,\rho}^{out}(A)$ is bounded as follows*

$$d_H(C(A), C_{r,\rho}^{out}(A)) \leq 9(2\rho_A + 1)^n \frac{r_A^2}{r^2}. \quad (6)$$

Proof. Any polynomial in $\mathbb{C}[c]_{r,\rho}$ can be written as $p(c) = w^* \phi(c)$, for some $w \in \mathbb{C}^N$ and with $\phi : \mathbb{C}^N \rightarrow \mathbb{C}^K$, where N is the number of Fourier coefficients up to harmonic degree ρ for functions on the torus T^n , i.e. $N = (2\rho + 1)^n$, while K is the number of Chebyshev polynomials up to degree r that we can build on \mathbb{C}^N , i.e. $K = \binom{r+N+1}{r}$. This representation allow us to identify $C_{r,\rho}^{out}(A)$ with $\widehat{\mathcal{K}}_s$ with $s = r$ and $C(A)$ with \mathcal{K}_s and $s = r$ from [5] and the use their Corollary 1 (note that we do not have a scale factor $1/(2r + 1)^d$).

Denote by $y(\mu) \in \mathbb{C}^K$ the vector of all the moments of a measure μ supported on the N Fourier coefficients up to algebraic degree r . By applying Corollary 1 of [5], we have that for any $\widehat{y} \in C_{r,\rho}^{out}$ there exists a measure μ supported on the N Fourier coefficients, such that

$$\|\Pi_r^{(r_A)}(\widehat{y} - y(\mu))\|_{\text{Fro}} \leq \frac{9Nr_A^2}{r^2},$$

where $\Pi_r^{(r_A)}$ is a diagonal matrix such that $(\Pi_r^{(r_A)})_{a,a} = 1$ iff a is the index of a Chebyshev polynomial with algebraic degree less or equal to r_A , otherwise it is $(\Pi_r^{(r_A)})_{a,a} = 0$. The proof is concluded by noting that $C(A) = \{\Pi_r^{(r_A)} y(\mu) \mid \mu \in M_\rho\}$, where M_ρ is the set of measures supported on Fourier coefficients with maximum harmonic degree ρ . \square

4.2 Inner approximations

Another approach consists of expressing measure ν as being absolutely continuous with respect to some reference measure γ whose moments can be easily calculated, e.g. the Gaussian measure on $\ell_2(\mathbb{Z}^n)$ [9].

Let

$$C_{r,\rho}^{\text{inn}}(A) := \{(y_{\mathbf{a}})_{\mathbf{a} \in A} : y_{\mathbf{a}} = \int_E c^{\mathbf{a}} p(c) d\gamma(c) \text{ for some } p \in Q_{r,\rho}\}.$$

Proposition 8. *For all $r, \rho \in \mathbb{N}$, $C_{r,\rho}^{\text{inn}}(A)$ is a semidefinite representable inner approximation of $C(A)$.*

Proof. The Radon-Nikodým derivative p of $\nu = p\gamma$ with respect to γ is constrained to the quadratic module $Q_{r,\rho}$, so that ν is non-negative on E . The proof is concluded by observing that y and p are related linearly, with p belonging to the semidefinite representable set $Q_{r,\rho}$. \square

Proposition 9. $\overline{C_{\infty,\infty}^{\text{inn}}}(A) = C(A)$.

Proof. As the proof of Proposition 6, according to Putinar's Positivstellensatz, elements of $Q_{r,\rho}$ can approximate as closely as desired any polynomial nonnegative

on E , i.e. we can construct a sequence $p_{r,\rho} \in Q_{r,\rho}$ such that $\|p - p_k\|_W \rightarrow 0$ when $r, \rho \rightarrow \infty$. It follows that for all $\mathbf{a} \in A$, $\int_E c^{\mathbf{a}} p_{r,\rho}(c) d\gamma(c) \rightarrow \int_E c^{\mathbf{a}} p(c) d\gamma(c) = y_{\mathbf{a}}$ when $r, \rho \rightarrow \infty$. \square

5 Solving Sobolev POPs

5.1 Harmonic Sobolev POP

We are now fully equipped to solve a harmonic Sobolev POP (polynomial optimization problem) of the form

$$p^* := \inf_{f \in B} p(f) \quad (7)$$

where

$$p(f) = \sum_{\mathbf{a} \in A} p_{\mathbf{a}} m_{\mathbf{a}}(f)$$

is a given Hermitian polynomial in the indeterminate $f \in B$, of support $A := \text{spt } p$. Problem (7) is called *harmonic* because the harmonic degree $\delta(p)$ is finite, and the problem does not involve harmonics of degrees higher than $\delta(p)$. Note that the infimum in (7) is always attained, since it is a finite-dimensional problem and B is bounded.

Harmonic Sobolev POP (7) is equivalent to the linear problem

$$p^* := \min_{\mu \in P(B)} \int_B p(f) d\mu(f)$$

on $P(B)$, the set of probability measures on the Sobolev ball B . Using the Fourier embedding, harmonic Sobolev POP (7) is equivalent to the harmonic Fourier POP

$$p^* := \min_{c \in E} p(c)$$

and the linear problem

$$p^* := \min_{\nu \in P(E)} \int_E p(c) d\nu(c)$$

on $P(E)$, the set of probability measures on the Fourier ellipsoid E . In turn, this is equivalent to the linear problem

$$p^* := \min_{y \in C(A)} \sum_{\mathbf{a} \in A} p_{\mathbf{a}} y_{\mathbf{a}} \text{ s.t. } y_{\emptyset} = 1 \quad (8)$$

on the cone of moments $C(A)$.

Therefore we can design a moment-SOS hierarchy of lower bounds

$$p_{r,\rho}^{\text{out}} := \min_{y \in C_{r,\rho}^{\text{out}}(A)} \sum_{\mathbf{a} \in A} p_{\mathbf{a}} y_{\mathbf{a}}$$

as well as a moment-SOS hierarchy of upper bounds

$$p_{r,\rho}^{\text{inn}} := \min_{y \in C_{r,\rho}^{\text{inn}}(A)} \sum_{\mathbf{a} \in A} p_{\mathbf{a}} y_{\mathbf{a}}$$

for increasing algebraic resp. harmonic relaxation degrees $r \geq d(p)$, $\rho \geq \delta(p)$.

Theorem 1. For all $r \geq r' \geq d(p)$ and $\rho \geq \rho' \geq \delta(p)$, it holds

$$p_{r',\rho'}^{\text{out}} \leq p_{r,\rho}^{\text{out}} \leq p_{\infty,\infty}^{\text{out}} = p^* = p_{\infty,\rho}^{\text{inn}} \leq p_{r,\rho}^{\text{inn}} \leq p_{r',\rho'}^{\text{inn}}.$$

Proof. It follows readily by applying Propositions 5, 6, 8 and 9. \square

5.1.1 Example

Consider the harmonic Sobolev POP

$$p^* = \min_{f \in B} \langle f, e_0 \rangle_{H^0(T)}^4 + (\langle f, e_1 \rangle_{H^0(T)}^2 - 1/4)^2$$

on $B \subset H^0(T)$, i.e. $n = 1$, $m = 0$ and harmonic degree $\rho = 1$. Observe that the function to be minimized is non-convex in f .

The harmonic Sobolev POP is equivalent to the harmonic Fourier POP

$$p^* = \min_{c_{-1}, c_0, c_1} c_0^4 + (c_1^2 - 1/4)^2 \text{ s.t. } c_{-1}^2 + c_0^2 + c_1^2 \leq 1.$$

Note that the Fourier coefficient c_{-1} does not appear in the objective function, and hence without loss of generality it can be set to zero. Alternatively, it may be desirable to penalize the higher degree Fourier coefficients with a quadratic regularization term.

With the outer moment-SOS hierarchy, at algebraic relaxation degree $r = 2$, we obtain the two global minimizers $c_{-1}^* = 0$, $c_0^* = 0$, $c_1^* = \pm 1/2$ and the corresponding functions $f^*(x) = \pm e^{-2\pi i x}/2$ achieving the global minimum $p^* = p_{2,1}^{\text{out}} = 0$.

5.2 Algebraic Sobolev POP

Another class of POP on Sobolev functions is

$$p^* = \inf_{f \in B} L(p(f, D^{a_1} f, \dots, D^{a_l} f)) \quad (9)$$

where p is a given real valued multivariate polynomial of degree d_p of a function $f \in B$ and its derivatives $D^{a_j} f$, $a_j \in \mathbb{N}^n$, $j = 1, \dots, l$ and $L : L^\infty(T^n) \rightarrow \mathbb{R}$ is a given bounded linear functional. Coefficients of p are bounded functions in x . For example

$$L(p(f)) = \int_{T^n} (p_1(x)f(x) + p_2(x)\|Df(x)\|_2^2) d\sigma(x) \quad (10)$$

where σ is a given probability measure on T^n and p_1, p_2 are given real polynomials of x .

Note that contrary to harmonic problem (7), the non-linearity hits directly the function value $f(x)$ and its derivatives, and hence problem (9) generally involves infinitely many harmonics. Still, problem (9) is called *algebraic* because p is a finite degree polynomial.

The following result guarantees that the non-linear functional defined above is well defined on $H^m(T^n)$ with m large enough.

Proposition 10. *The functional of Sobolev POP (9) is bounded when $f \in H_2^{s+n/2+1}(T^n)$ where $s = \max_{j=1,\dots,k} |a_j|$.*

Proof. By the Sobolev embedding theorem [1] in a bounded set Ω with Lipschitz boundary in \mathbb{R}^n , when $f \in H_2^{m+n/2+1}(\Omega)$ then $D^a f$ is a Lipschitz function for any a satisfying $|a| \leq m$. Since now $D^{a_j} f \in L^q(\Omega)$ for any $q \in [1, \infty]$ (due to the boundedness of Ω), the desired result is obtained by applying the Hölder inequality. \square

Let us express the objective function of (9) as a polynomial function of c , the Fourier coefficients of f . Indeed, if $f = \langle c, e \rangle_{\ell_2} = \sum_{a \in \mathbb{Z}^n} c_a e_{-a}$ then a monomial of degree $d \in \mathbb{N}$ writes

$$f^d = \langle c, e \rangle_{\ell_2}^d = \sum_{a_1, a_2, \dots, a_d \in \mathbb{Z}^n} c_{a_1} c_{a_2} \cdots c_{a_d} e_{-(a_1 + a_2 + \dots + a_d)}$$

and it follows that

$$L(f^d) = \sum_{a_1, a_2, \dots, a_d \in \mathbb{Z}^n} c_{a_1} c_{a_2} \cdots c_{a_d} z_{-(a_1 + a_2 + \dots + a_d)}$$

where $z_a := L(e_a)$ is the moment of index $a \in \mathbb{Z}^n$ of linear functional L . Similarly, successive derivatives of f will be expressed as linear functions of c , and hence polynomials of these derivatives will be multivariate polynomials of c . Overall, the objective function is a polynomial q in infinitely countably many variables with finite algebraic degree $d(q) = d_p$ and infinite harmonic degree $\delta(q) = \infty$. Algebraic Sobolev POP (9) can therefore be written equivalently as the algebraic Fourier POP

$$p^* = \inf_{c \in E} q(c) = \sum_{\mathbf{a} \in \mathbb{Z}^n} q_{\mathbf{a}} c^{\mathbf{a}}.$$

In order to apply the moment-SOS hierarchy, we reformulate this POP as a linear problem

$$p^* := \min_{\nu \in P(E)} \int_E q(c) d\nu(c)$$

on $P(E)$, the set of probability measures on the Fourier ellipsoid E . In turn, this is equivalent to the infinite-dimensional linear problem

$$p^* := \min_{y \in C(\mathbb{Z}^n)} \sum_{\mathbf{a} \in \mathbb{Z}^n} q_{\mathbf{a}} y_{\mathbf{a}} \text{ s.t. } y_{\emptyset} = 1$$

on the full cone of moments

$$C(\mathbb{Z}^n) := \{(y_{\mathbf{a}})_{\mathbf{a} \in \mathbb{Z}^n} : y_{\mathbf{a}} = \int_E c^{\mathbf{a}} d\nu(c) \text{ for some } \nu \text{ supported on } E\} \in \ell_2(\mathbb{Z}^n).$$

In contrast, the harmonic Sobolev POP of the previous section was reformulated as the finite-dimensional linear problem (8) on a truncated cone of moments.

As in the previous section, for every finite algebraic resp. harmonic degrees r and ρ , we can define the outer approximations

$$C_{r,\rho}^{\text{out}}(\mathbb{Z}^n) := \Pi_A\{(y_{\mathbf{a}})_{\mathbf{a} \in \mathbb{Z}^n} : \ell_y(q) = \sum_{\mathbf{a} \in \mathbb{Z}^n} q_{\mathbf{a}} c^{\mathbf{a}} \geq 0 \text{ for all } q \in Q_{r,\rho}\}$$

and inner approximations

$$C_{r,\rho}^{\text{inn}}(\mathbb{Z}^n) := \{(y_{\mathbf{a}})_{\mathbf{a} \in \mathbb{Z}^n} : y_{\mathbf{a}} = \int_E c^{\mathbf{a}} q(c) d\gamma(c) \text{ for some } q \in Q_{r,\rho}\}$$

such that $C_{r,\rho}^{\text{inn}}(\mathbb{Z}^n) \subset C(\mathbb{Z}^n) \subset C_{r,\rho}^{\text{out}}(\mathbb{Z}^n)$ and asymptotically $\overline{C_{\infty,\infty}^{\text{inn}}(\mathbb{Z}^n)} = C(\mathbb{Z}^n) = \overline{C_{\infty,\infty}^{\text{out}}(\mathbb{Z}^n)}$, but these are now infinite-dimensional cones that must be truncated to be manipulated numerically.

Given algebraic resp. harmonic degrees r and ρ , let us consider the finite-dimensional linear problem

$$p_{r,\rho}^* := \min_{y \in C(A_{r,\rho})} \sum_{\mathbf{a} \in A_{r,\rho}} q_{\mathbf{a}} y_{\mathbf{a}} \text{ s.t. } y_{\emptyset} = 1$$

on the finite-dimensional cone of moments $C(A_{r,\rho})$ indexed by

$$A_{r,\rho} := \{\mathbf{a} \in \mathbb{Z}^n : d_{\mathbf{a}} \leq r, \delta_{\mathbf{a}} \leq \rho\}.$$

We can design an outer moment-SOS hierarchy of lower bounds

$$p_{r,\rho}^{\text{out}} := \min_{y \in C_{r,\rho}^{\text{out}}(A_{r,\rho})} \sum_{\mathbf{a} \in A_{r,\rho}} q_{\mathbf{a}} y_{\mathbf{a}}$$

as well as an inner moment-SOS hierarchy of upper bounds

$$p_{r,\rho}^{\text{inn}} := \min_{y \in C_{r,\rho}^{\text{inn}}(A_{r,\rho})} \sum_{\mathbf{a} \in A_{r,\rho}} q_{\mathbf{a}} y_{\mathbf{a}}$$

for increasing algebraic resp. harmonic relaxation degrees r and ρ . Our convergence result then follows immediately from the above considerations.

Theorem 2. *For finite r, ρ it holds $p_{r,\rho}^{\text{out}} \leq p_{r,\rho}^* \leq p_{r,\rho}^{\text{inn}}$. Asymptotically it holds $p_{\infty,\infty}^{\text{out}} = p^* = p_{\infty,\infty}^{\text{inn}}$.*

5.2.1 Example

Consider the algebraic Sobolev POP

$$p^* = \inf_{f \in B} \int_T (f(x)^2 - 1/2)^2 d\sigma(x)$$

where σ is the Dirac measure at 0 on $B \subset H^0(T)$, i.e. $m = 0$ and $n = 1$. Observe that the function to be minimized is non-convex in f .

Since $f(0) = \sum_{a \in \mathbb{Z}} c_a$, the moments z_a of the linear functional in the objective function are equal to one for all $a \in \mathbb{Z}$ so the problem can be written as the algebraic Fourier POP

$$p^* = \inf_{c \in E} q(c)$$

with

$$q(c) = \frac{1}{4} - \sum_{a_1, a_2 \in \mathbb{Z}} c_{a_1} c_{a_2} + \sum_{a_1, a_2, a_3, a_4 \in \mathbb{Z}} c_{a_1} c_{a_2} c_{a_3} c_{a_4}.$$

With the outer moment-SOS hierarchy, at algebraic relaxation degree $r = 2$ and harmonic relaxation degree $\rho = 0$, we obtain the two global minimizers $c_0^* = \pm\sqrt{2}/2$ and the corresponding functions $f^*(x) = \pm\sqrt{2}/2$ achieving the global minimum $p^* = p_{2,0}^{\text{out}} = 0$.

Note that for such problems it may be desirable to penalize the higher degree Fourier coefficients with a quadratic regularization term.

5.3 Kernel Sobolev POP

While an algebraic Sobolev POP generally requires an infinite number of Fourier coefficients to be expressed, actually there exists a better basis, based on *kernel methods* [4], where the problem admits a representation in terms of a finite number of coefficients. Since $H^m(T^n)$ is a *reproducing kernel Hilbert space* when $m > n/2$, there exists a kernel function $k : T^n \times T^n \rightarrow \mathbb{R}$ such that $k(x, y) = k(y, x)$, $k(\cdot, x) \in H^m(T^n)$ for any $x, y \in T^n$ and more importantly, we have the reproducing property: for any $f \in H^m(T^n)$ and any $x \in T^n$, the following holds

$$f(x) = \langle f, k(\cdot, x) \rangle_{H^m(T^n)}.$$

In particular, for the case of $H^m(T^n)$ the kernel is known in closed form in terms of the Bessel function of the second kind, see [7, Sec. 7.4]. Then the powerful and fundamental result in machine learning known as the Representer Theorem [31] holds.

Theorem 3. *The Sobolev POP*

$$\min_{f \in H^m(T^n)} p(f(x_1), \dots, f(x_l)) \quad (11)$$

for a given polynomial p is equivalent to the finite-dimensional POP

$$\min_{w \in \mathbb{R}^l} p(\langle c_1, w \rangle_{\mathbb{R}^l}, \dots, \langle c_n, w \rangle_{\mathbb{R}^l}) \quad (12)$$

where $c_j := (k(x_i, x_j))_{i=1, \dots, l}$, $j = 1, \dots, l$. The first problem admits a solution and only if the second problem admits a solution, and both problems have the same value. In particular, denoting by f^* the solution of the first problem and w^* the solution of the second problem, we have

$$f^*(\cdot) = \sum_{j=1}^l w_j^* k(\cdot, x_j).$$

More generally, the Sobolev POP

$$\min_{f \in H^m(T^n)} p(\langle g_1, f \rangle_{H^m(T^n)}, \dots, \langle g_l, f \rangle_{H^m(T^n)}) \quad (13)$$

for a given polynomial p and given $g_j \in H^{-m}(T^n)$ is equivalent to the finite-dimensional POP (12) where $c_j = (\langle g_i, g_j \rangle_{H^m(T^n)})_{i=1, \dots, l}$, $j = 1, \dots, l$ and

$$f^* = \sum_{j=1}^l w_j^* g_j.$$

Note that POP (11) is a particular case of POP (13) corresponding to the choice $g_j(\cdot) = k(\cdot, x_j)$ since $\langle f, k(\cdot, x_j) \rangle_{H^m(T^n)} = f(x_j)$, $j = 1, \dots, l$.

Theorem 3 implies that for kernel Sobolev POPs of the form (13), we can apply the standard finite-dimensional moment-SOS hierarchy [19] with convergence guarantees.

Note that Theorem 3 also holds when p is any continuous function which is bounded below (not necessarily a polynomial), for any measurable space X beyond T^n , and any space of functions on X that is a reproducing kernel Hilbert space, for example any Sobolev space $H^m(X)$ where $X \subseteq \mathbb{R}^n$ is a domain with locally Lipschitz boundary and $m > n/2$.

5.3.1 Example

Revisiting Example 5.2.1, since the objective function is $(f(0)^2 - 1/2)^2$, i.e. $p(t) = (t^2 - 1/2)^2$ and $x_1 = 0$, $l = 1$ in Sobolev POP (11), it can be expressed equivalently as the univariate POP $\min_{w_1 \in \mathbb{R}} (w_1^2 k(0, 0)^2 - 1/2)^2$ whose solutions are $w_1 = \pm \frac{\sqrt{2}}{2k(0, 0)}$, corresponding to the following minimizers $f^*(x) = \pm \frac{\sqrt{2}k(x, 0)}{2k(0, 0)}$.

6 Solution recovery

When solving infinite-dimensional calculus of variations of control problems, we may be faced with truncated moment problems on Sobolev spaces with an increasing number of Fourier coefficients. When the number of Fourier coefficients goes to infinity, we know that there is a single representing measure, i.e. the infinite-dimensional moment problem is determinate.

Proposition 11. *A measure μ supported on B is uniquely determined by its infinite-dimensional sequence of moments $(y_{\mathbf{a}})_{\mathbf{a} \in c_0(\mathbb{Z}^n)}$.*

Proof. The sequence of moments $(y_{\mathbf{a}})_{\mathbf{a} \in c_0(\mathbb{Z}^n)}$ in (5) exists and is unique with respect to ν , since ν is a measure defined on E which is a compact Hausdorff set, and the function $m_{\mathbf{a}}(c)$ is a monomial in the coefficients c . So we can apply the Stone–Weierstrass theorem. To conclude, note that ν and μ are in one-to-one relation via the invertible linear map F , recall (3). \square

Given a sequence of moments, we may want to recover the representing measure on B . In the finite-dimensional case, the Christoffel-Darboux kernel can be used to approximate the support of a measure given its moments [20]. It would be interesting to extend this kernel to Sobolev spaces.

7 Conclusion

In this paper we address and solve numerically the moment problem for measures supported on the unit ball of a Sobolev space. We describe how the finite-dimensional moment-SOS hierarchy can be extended to this infinite-dimensional setup, allowing to solve numerically polynomial optimization problems on Sobolev spaces while preserving approximation and convergence guarantees.

All our developments are done for a specific basis of complex exponentials (1), but similar results could be achieved for any basis with good approximation properties for the Sobolev space $H^m(T^n)$ or other reproducing kernel Hilbert spaces, as highlighted in Section 5.3.

Our approach can also be generalized with the exact same construction to other spaces like Sobolev spaces on general domains, Besov or Triebel-Lizorkin spaces and more generally quasi-Banach spaces where there exists a Schauder basis with reasonable approximation properties.

Finally, applications of these techniques and the infinite-dimensional moment-SOS hierarchy to the approximation of solutions of nonlinear calculus of variations problems or optimal control involving non-linear partial differential equations remain to be investigated.

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